

# Hamiltonian integration methods for Vlasov-Maxwell equations

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## Abstract

Hamiltonian integration methods for the Vlasov-Maxwell equations are developed by a Hamiltonian splitting technique. The Hamiltonian functional is split into five parts, i.e., the electrical energy, the magnetic energy, and the kinetic energy in three Cartesian components. Each of the subsystems is a Hamiltonian system with respect to the Morrison-Marsden-Weinstein Poisson bracket and can be solved exactly. Compositions of the exact solutions yield Poisson structure preserving, or Hamiltonian, integration methods for the Vlasov-Maxwell equations, which have superior long-term fidelity and accuracy.

The dynamics of charged particles in a plasma interacting with the self-consistent electromagnetic fields can be described by the Vlasov-Maxwell (VM) equations. In modern plasma physics and accelerator physics, numerical integration of the Vlasov-Maxwell equations is an important tool for theoretical studies, and varieties of numerical algorithms have been developed. Recently, geometric integration methods [1–4], which are designed in the spirit of preserving the intrinsic structures of a dynamical system, have been developed for plasma physics applications [5–19]. By preserving properties such as the Poisson structure of a Hamiltonian system and the invariant volume form of a source-free system, geometric integration methods usually generate numerical results with superior long-term behavior compared to other methods [4, 20], and are thus more suitable for large-scale, long-term simulations. It is known that the Vlasov-Maxwell system is a Hamiltonian system with respect to a Poisson bracket [21–23]. In a recent paper [18], Crouseilles, Einkemmer, and Faou proposed an innovative Hamiltonian splitting method for the Vlasov-Maxwell equations based on a bracket first suggested in Ref. [21]. This splitting scheme results in three solvable subsystems, whose exact solutions can be combined into algorithms for the Vlasov-Maxwell equations that preserve the structure specified by the bracket. However, it has been pointed out in Ref. [24] that the bracket adopted in Ref. [18] is not Poisson, because it does not satisfy the Jacobi identity [22, 23]. Very disappointedly, if the Hamiltonian splitting method proposed in Ref. [18] is applied with the correct Poisson bracket, a.k.a. the Morrison-Marsden-Weinstein (MMW) bracket [22–25], one of the subsystems cannot be solved exactly in general. Therefore, Hamiltonian integration methods for the Vlasov-Maxwell equations cannot be constructed by using the splitting method developed in Ref. [18].

In this paper, we apply the MMW Poisson bracket [22, 23] and develop a family of Hamiltonian integration methods via a new splitting of the Hamiltonian functional. In the current context, a Hamiltonian integration method is defined as a numerical integrator that preserves the Poisson structure of the Vlasov-Maxwell system specified by the MMW bracket. In addition to splitting the Hamiltonian into electrical energy, magnetic energy, and kinetic energy, we further split the kinetic energy into three Cartesian components. It turns out that exact solutions for all of the resulted subsystems can be calculated by the method of characteristics. By compositions of the exact solutions to the subsystems, methods of theoretically arbitrarily high order in time for the original Vlasov-Maxwell equations can be constructed. The exact solutions of the subsystems preserve the same Poisson structure

as the Vlasov-Maxwell equations, so do the combined algorithms. Therefore, the good properties of a Hamiltonian integrator, such as the long-term stability and accuracy and global bound on the energy error, are all inherited by this family of new integration methods for the Vlasov-Maxwell system.

The Vlasov-Maxwell equations considered in the present study are

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} = 0, \quad (1)$$

$$\nabla \times \mathbf{B} = \int \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} + \frac{\partial \mathbf{E}}{\partial t}, \quad (2)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad (3)$$

$$\nabla \cdot \mathbf{E} = \int f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}, \quad (4)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (5)$$

where  $f(\mathbf{x}, \mathbf{v}, t)$  is the distribution function of position  $\mathbf{x} \in U \subset \mathbb{R}^3$  and velocity  $\mathbf{v} \in \mathbb{R}^3$  at time  $t$ , and  $(\mathbf{E}(\mathbf{x}, t), \mathbf{B}(\mathbf{x}, t)) \in \mathbb{R}^3 \times \mathbb{R}^3$  are the electromagnetic fields. For easy presentation, the species index, charge, mass, and other constant are omitted. Equations (1)-(3) are closed, and equations (4)-(5) result from the gauge symmetry of the system. According to [23], the VM equations (1)-(5) are equivalent to the Hamiltonian system

$$\frac{\partial \mathcal{F}}{\partial t} = \{\{\mathcal{F}, \mathcal{H}\}\} \quad (6)$$

on the phase space  $\mathcal{MV} = \{(\mathbf{E}, \mathbf{B}) | \nabla \cdot \mathbf{B} = 0, \nabla \cdot \mathbf{E} = \int f d\mathbf{v}\}$ , with  $\mathcal{F}(f, \mathbf{E}, \mathbf{B})$  being any functional on  $\mathcal{MV}$  and  $\mathcal{H}$  being the Hamiltonian functional defined as

$$\mathcal{H}(f, \mathbf{E}, \mathbf{B}) = \frac{1}{2} \int |\mathbf{v}|^2 f(\mathbf{x}, \mathbf{v}, t) d\mathbf{x} d\mathbf{v} + \frac{1}{2} \int (|\mathbf{E}(\mathbf{x}, t)|^2 + |\mathbf{B}(\mathbf{x}, t)|^2) d\mathbf{x}. \quad (7)$$

Here,  $\{\{\cdot, \cdot\}\}$  denotes the Morrison-Marsden-Weinstein bracket [21–23],

$$\begin{aligned} \{\{\mathcal{F}, \mathcal{G}\}\}(f, \mathbf{E}, \mathbf{B}) &= \int f \left\{ \frac{\delta \mathcal{F}}{\delta f}, \frac{\delta \mathcal{G}}{\delta f} \right\}_{\mathbf{xv}} d\mathbf{x} d\mathbf{v} \\ &+ \int \left[ \frac{\delta \mathcal{F}}{\delta \mathbf{E}} \cdot \left( \nabla \times \frac{\delta \mathcal{G}}{\delta \mathbf{B}} \right) - \frac{\delta \mathcal{G}}{\delta \mathbf{E}} \cdot \left( \nabla \times \frac{\delta \mathcal{F}}{\delta \mathbf{B}} \right) \right] d\mathbf{x} \\ &+ \int \left( \frac{\delta \mathcal{F}}{\delta \mathbf{E}} \cdot \frac{\partial f}{\partial \mathbf{v}} \frac{\delta \mathcal{G}}{\delta f} - \frac{\delta \mathcal{G}}{\delta \mathbf{E}} \cdot \frac{\partial f}{\partial \mathbf{v}} \frac{\delta \mathcal{F}}{\delta f} \right) d\mathbf{x} d\mathbf{v} \\ &+ \int f \mathbf{B} \cdot \left( \frac{\partial}{\partial \mathbf{v}} \frac{\delta \mathcal{F}}{\delta f} \times \frac{\partial}{\partial \mathbf{v}} \frac{\delta \mathcal{G}}{\delta f} \right) d\mathbf{x} d\mathbf{v}. \end{aligned} \quad (8)$$

In the first term on the right-hand side,  $\{\cdot, \cdot\}_{\mathbf{x}\mathbf{v}}$  denotes the canonical Poisson bracket for functions of  $(\mathbf{x}, \mathbf{v})$ . With the initial conditions  $f(\mathbf{x}, \mathbf{v}, 0) = f_0(\mathbf{x}, \mathbf{v})$  and  $(\mathbf{E}(\mathbf{x}, 0), \mathbf{B}(\mathbf{x}, 0)) \in \mathcal{MV}$ , there exists unique solution to the system (6), on which the bracket (8) is Poisson and is preserved. Given this Hamiltonian formulation of the Vlasov-Maxwell system, Poisson structure preserving integration methods can be constructed as follows. The system is first split into several solvable subsystems by decomposing the Hamiltonian functional (7). We then find the exact solutions to the subsystems, and finally the exact solutions of the subsystems are composed in a proper way to construct integrators for the Vlasov-Maxwell equations that preserve the Poisson structure (8).

Firstly, we follow Ref. [18] to split the Hamiltonian into three parts,

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_E + \mathcal{H}_B + \mathcal{H}_f, \\ \mathcal{H}_E &= \frac{1}{2} \int |\mathbf{E}(\mathbf{x}, t)|^2 d\mathbf{x}, \quad \mathcal{H}_B = \frac{1}{2} \int |\mathbf{B}(\mathbf{x}, t)|^2 d\mathbf{x}, \quad \mathcal{H}_f = \frac{1}{2} \int |\mathbf{v}|^2 f(\mathbf{x}, \mathbf{v}, t) d\mathbf{x} d\mathbf{v}. \end{aligned} \quad (9)$$

Using the MMW bracket (8) and the Hamiltonian equation (6), the VM equations (1)-(5) can be split into three subsystems on  $\mathcal{MV}$ ,

$$\dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_E\}\}, \quad \dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_B\}\}, \quad \dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_f\}\}.$$

Next, we try to solve the subsystems for exact solutions. The subsystem  $\dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_E\}\}$  associated with the Hamiltonian  $\mathcal{H}_E$  is equivalent to

$$\begin{aligned} \frac{\partial f}{\partial t} + \mathbf{E}(\mathbf{x}, t) \cdot \frac{\partial f}{\partial \mathbf{v}} &= 0, \\ \frac{\partial \mathbf{E}}{\partial t} &= 0, \\ \frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \mathbf{E}. \end{aligned} \quad (10)$$

Given the initial functions  $f_0$  and  $(\mathbf{E}(\mathbf{x}, 0), \mathbf{B}(\mathbf{x}, 0)) \in \mathcal{MV}$ , the solution to the subsystem (10) is

$$\begin{aligned} f(\mathbf{x}, \mathbf{v}, t) &= f_0(\mathbf{x}, \mathbf{v} - t\mathbf{E}(\mathbf{x}, 0)), \\ \mathbf{E}(\mathbf{x}, t) &= \mathbf{E}(\mathbf{x}, 0), \\ \mathbf{B}(\mathbf{x}, t) &= \mathbf{B}(\mathbf{x}, 0) - t\nabla \times \mathbf{E}(\mathbf{x}, 0). \end{aligned} \quad (11)$$

Using the notation  $\exp(\mathcal{H}_E t)$  as the update operator in time, we denote this solution formally as

$$(f(\mathbf{x}, \mathbf{v}, t), \mathbf{E}(\mathbf{x}, t), \mathbf{B}(\mathbf{x}, t))^T = \exp(\mathcal{H}_E t)(f_0(\mathbf{x}, \mathbf{v}), \mathbf{E}(\mathbf{x}, 0), \mathbf{B}(\mathbf{x}, 0))^T.$$

The subsystem  $\dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_B\}\}$  corresponding to the Hamiltonian  $\mathcal{H}_B$  is equivalent to,

$$\begin{aligned}\frac{\partial f}{\partial t} &= 0, \\ \frac{\partial \mathbf{E}}{\partial t} &= \nabla \times \mathbf{B}, \\ \frac{\partial \mathbf{B}}{\partial t} &= 0.\end{aligned}\tag{12}$$

With initial conditions given on  $\mathcal{MV}$ , the solution to the subsystem (12) is

$$\begin{aligned}f(\mathbf{x}, \mathbf{v}, t) &= f_0(\mathbf{x}, \mathbf{v}), \\ \mathbf{E}(\mathbf{x}, t) &= \mathbf{E}(\mathbf{x}, 0) + t\nabla \times \mathbf{B}(\mathbf{x}, 0), \\ \mathbf{B}(\mathbf{x}, t) &= \mathbf{B}(\mathbf{x}, 0).\end{aligned}\tag{13}$$

We denote the corresponding update operator as  $\exp(\mathcal{H}_B t)$ .

For the Hamiltonian  $\mathcal{H}_f$ , however, the subsystem  $\dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_f\}\}$  is in a more complicated form,

$$\begin{aligned}\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + (\mathbf{v} \times \mathbf{B}(\mathbf{x}, t)) \cdot \frac{\partial f}{\partial \mathbf{v}} &= 0, \\ \frac{\partial \mathbf{E}}{\partial t} &= - \int \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}, \\ \frac{\partial \mathbf{B}}{\partial t} &= 0.\end{aligned}\tag{14}$$

It has been shown that unless the magnetic field  $\mathbf{B}$  vanishes or is uniform in space, this system can not be solved exactly [24]. Therefore, we search for a Poisson structure preserving method for Eq. (14) by further splitting the Hamiltonian  $\mathcal{H}_f$  into more solvable subsystems. Utilizing the structure of the cross product in the Cartesian frame,

$$\mathbf{v} \times \mathbf{B} = \hat{\mathbf{B}}\mathbf{v} = \begin{bmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{bmatrix} \mathbf{v},$$

we further split the Hamiltonian  $\mathcal{H}_f$  into different Cartesian components, i.e.,

$$\mathcal{H}_f = \mathcal{H}_{1f} + \mathcal{H}_{2f} + \mathcal{H}_{3f}, \quad \mathcal{H}_{if} = \frac{1}{2} \int v_i^2 f(\mathbf{x}, \mathbf{v}, t) d\mathbf{x} d\mathbf{v}, \quad i = 1, 2, 3.\tag{15}$$

The subscript of  $B$  and  $v$  denotes the corresponding Cartesian component of the vector.

The subsystem associated with each Hamiltonian  $\mathcal{H}_{if}$  is

$$\begin{aligned} \frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} - B_{i-1}(\mathbf{x}) v_i \frac{\partial f}{\partial v_{i+1}} + B_{i+1}(\mathbf{x}) v_i \frac{\partial f}{\partial v_{i-1}} &= 0, \\ \frac{\partial E_i}{\partial t} &= - \int v_i f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}, \\ \frac{\partial \mathbf{B}}{\partial t} &= 0, \quad \frac{\partial E_{i-1}}{\partial t} = \frac{\partial E_{i+1}}{\partial t} = 0, \end{aligned} \tag{16}$$

with  $v_4 := v_1$  and  $v_0 := v_3$ . The first equation of (16) can be solved by the method of characteristics, and the characteristic equations are

$$\dot{x}_i = v_i, \quad \dot{v}_{i+1} = -B_{i-1}(\mathbf{x})v_i, \quad \dot{v}_{i-1} = B_{i+1}(\mathbf{x})v_i.$$

It is a system of ordinary differential equations, whose exact solution is

$$\begin{aligned} x_i(t) &= x_i(0) + tv_i, \\ v_{i+1}(t) &= v_{i+1}(0) - \int_{x_i(0)}^{x_i(t)} B_{i-1}(\mathbf{x}) dx_i, \\ v_{i-1}(t) &= v_{i-1}(0) + \int_{x_i(0)}^{x_i(t)} B_{i+1}(\mathbf{x}) dx_i. \end{aligned}$$

Therefore, for the initial conditions  $f(\mathbf{x}, \mathbf{v}, 0) = f_0(\mathbf{x}, \mathbf{v})$  and  $(\mathbf{E}(\mathbf{x}, 0), \mathbf{B}(\mathbf{x}, 0)) \in \mathcal{MV}$ , the exact solution to the subsystem (16) is

$$\begin{aligned} f(\mathbf{x}, \mathbf{v}, t) &= f_0(\mathbf{x} - tv_i \mathbf{e}_i, \mathbf{v} + F_{i-1} \mathbf{e}_{i+1} - F_{i+1} \mathbf{e}_{i-1}), \\ F_l &= \int_{x_i - tv_i}^{x_i} B_l(\mathbf{x}) dx_i, \quad l = i+1, i-1, \\ \mathbf{E}(\mathbf{x}, t) &= \mathbf{E}(\mathbf{x}, 0) - \int_0^t \int \mathbf{e}_i v_i f(\mathbf{x}, \mathbf{v}, \tau) d\mathbf{v} d\tau, \\ \mathbf{B}(\mathbf{x}, t) &= \mathbf{B}(\mathbf{x}, 0), \end{aligned} \tag{17}$$

where  $\mathbf{e}_i$  is the unit vector in the  $i$ -th Cartesian direction. We denote the exact solution given by Eq. (17) as  $(f, \mathbf{E}, \mathbf{B})(t)^T = \exp(\mathcal{H}_{if}t)(f_0(\mathbf{x}, \mathbf{v}), \mathbf{E}(\mathbf{x}, 0), \mathbf{B}(\mathbf{x}, 0))^T$ . More specifically, the exact solution of the subsystem corresponding to  $\mathcal{H}_{1f}$  is

$$\begin{aligned} f(\mathbf{x}, \mathbf{v}, t) &= f_0(x_1 - tv_1, x_2, x_3, v_1, v_2 + v_1 F_3, v_3 - v_1 F_2), \\ F_l &= \int_{x_1 - tv_1}^{x_1} B_l(\mathbf{x}) dx_1, \quad l = 2, 3, \\ E_1(\mathbf{x}, t) &= E_1(\mathbf{x}, 0) - \int_0^t \int v_1 f(\mathbf{x}, \mathbf{v}, \tau) d\mathbf{v} d\tau. \end{aligned}$$

The exact solution associated with  $\exp(\mathcal{H}_{2f}t)$  is

$$\begin{aligned} f(\mathbf{x}, \mathbf{v}, t) &= f_0(x_1, x_2 - tv_2, x_3, v_1 - v_2 F_3, v_2, v_3 + v_2 F_1), \\ F_l &= \int_{x_2 - tv_2}^{x_2} B_l(\mathbf{x}) dx_2, l = 1, 3, \\ E_2(\mathbf{x}, t) &= E_2(\mathbf{x}, 0) - \int_0^t \int v_2 f(\mathbf{x}, \mathbf{v}, \tau) d\mathbf{v} d\tau, \end{aligned}$$

and the exact solution associated with  $\exp(\mathcal{H}_{3f}t)$  is

$$\begin{aligned} f(\mathbf{x}, \mathbf{v}, t) &= f_0(x_1, x_2, x_3 - tv_3, v_1 + v_3 F_2, v_2 - v_3 F_1, v_3), \\ F_l &= \int_{x_3 - tv_3}^{x_3} B_l(\mathbf{x}) dx_3, l = 1, 2, \\ E_3(\mathbf{x}, t) &= E_3(\mathbf{x}, 0) - \int_0^t \int v_3 f(\mathbf{x}, \mathbf{v}, \tau) d\mathbf{v} d\tau. \end{aligned}$$

Overall, we split the Vlasov-Maxwell equations into five subsystems,

$$\mathcal{H} = \mathcal{H}_E + \mathcal{H}_B + \mathcal{H}_{1f} + \mathcal{H}_{2f} + \mathcal{H}_{3f},$$

$$\dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_E\}\}, \dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_B\}\}, \dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_{1f}\}\}, \dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_{2f}\}\}, \dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}_{3f}\}\}.$$

with  $\mathcal{H}_E, \mathcal{H}_B$  and  $\mathcal{H}_{if}, i = 1, 2, 3$ , defined in Eqs. (9) and (15), and the Poisson bracket being defined in Eq. (8). The exact solutions to the subsystems are given explicitly by Eqs. (11), (13), and (17), respectively. For initial functions defined on  $\mathcal{MV}$ , the solutions of the subsystems are all on  $\mathcal{MV}$  and preserve the MMW Poisson bracket.

Given exact solutions to the subsystems, integration methods for the original Vlasov-Maxwell equations can be constructed by compositions. For example, if we denote the solution at time  $t$  as  $Z(t) := (f(\mathbf{x}, \mathbf{v}, t), \mathbf{E}(\mathbf{x}, t), \mathbf{B}(\mathbf{x}, t))^T$ , a first order numerical update in one time step with step size  $\Delta t$  can be derived from the Lie-Trotter composition

$$Z(t + \Delta t) = \exp(\Delta t \mathcal{H}_E) \exp(\Delta t \mathcal{H}_B) \exp(\Delta t \mathcal{H}_{1f}) \exp(\Delta t \mathcal{H}_{2f}) \exp(\Delta t \mathcal{H}_{3f}) Z(t),$$

and a second order symmetric method can be constructed by the following symmetric composition,

$$\begin{aligned} Z(t + \Delta t) = & \exp\left(\frac{\Delta t}{2} \mathcal{H}_E\right) \exp\left(\frac{\Delta t}{2} \mathcal{H}_B\right) \exp\left(\frac{\Delta t}{2} \mathcal{H}_{1f}\right) \exp\left(\frac{\Delta t}{2} \mathcal{H}_{2f}\right) \exp(\Delta t \mathcal{H}_{3f}) \\ & \exp\left(\frac{\Delta t}{2} \mathcal{H}_{2f}\right) \exp\left(\frac{\Delta t}{2} \mathcal{H}_{1f}\right) \exp\left(\frac{\Delta t}{2} \mathcal{H}_B\right) \exp\left(\frac{\Delta t}{2} \mathcal{H}_E\right) Z(t). \end{aligned}$$

With the help of the BCH formula, proper compositions can be found to yield methods of arbitrarily high order in time [4, 26]. Given the geometrical properties of the solutions to the subsystems, the combined methods will preserve the Poisson structure and generate solutions on  $\mathcal{MV}$ , if the initial values  $Z(0)$  are taken on  $\mathcal{MV}$ .

In conclusion, we have constructed a family of Poisson structure preserving, or Hamiltonian, integration methods for the Vlasov-Maxwell equations by the splitting technique. The Hamiltonian is split into five parts, each part associates with a solvable Hamiltonian subsystem with respect to the MMW Poisson bracket. As a consequence, integration methods for the Vlasov-Maxwell equations constructed via composition of the exact solutions of the subsystems will preserve the original Poisson structure. These new Hamiltonian methods are expected to exhibit long-term accuracy and fidelity, as well as bounded error in energy and other invariants. Numerical applications of the methods will be reported in future publications.

In the present study, we have focused on the time integration of the Vlasov-Maxwell system and the preservation of the original Poisson structure. If the system is discretized in space, the resulted scheme needs to preserve a discrete Poisson bracket depending on the spatial discretization scheme [19].

As a final note, we emphasize that this general methodology of constructing Hamiltonian integration algorithms via Hamiltonian splitting is also applicable to other systems that admit Poisson structures. Recently, Burby et al. discovered the Poisson structures for the gyrokinetic system [25] and the collision operator [27]. Application of the splitting technique to these systems will generate more effective numerical algorithms for large-scale, long-term simulation studies of plasma physics.

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